

# The Terascale Simulation Tools and Technologies Center



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<http://www.tsstt-scidac.org/>

Terascale  
Simulation  
Tools  
and  
Technologies

**TSTT**

# The TSTT Center

- *Goal:* To enable high-fidelity calculations based on multiple coupled physical processes and multiple physical scales
  - *Adaptive methods*
  - *Composite or hybrid solution strategies*
  - *High-order discretization strategies*
- *Barrier:* The lack of easy-to-use interoperable meshing, discretization, and adaptive tools requires too much software expertise by application scientists

*The TSTT center recognizes this gap and will address the technical and human barriers preventing use of adaptive, composite, hybrid methods*

# TSTT Participants

- ANL: *Fischer*, Leurent, Tufo
- BNL: *Glimm*, Samulyak
- LLNL: *Brown*, Chand, Fast, Henshaw, Quinlan
- ORNL: *D' Azevedo*, de Almeida, Khamayseh
- PNNL: *Trease*
- RPI: Flaherty, Hau, Remacle, *Shephard*
- SNL: Brewer, Freitag, *Knupp*, Melander, Tautges
- SUNY SB: Glimm, *Li*

*\*Italics: site PI*

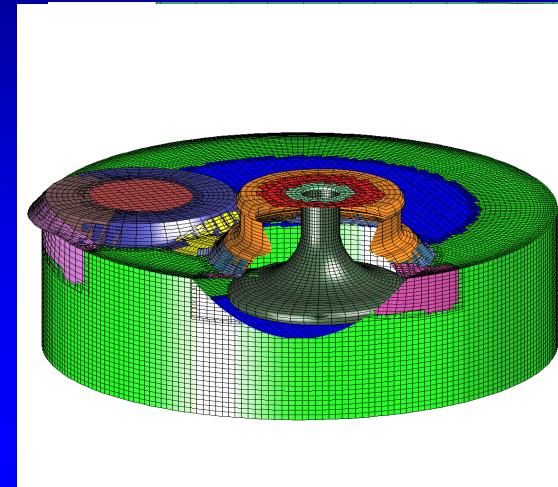
# TSTT Mesh Management Tools

- **Structured meshes**

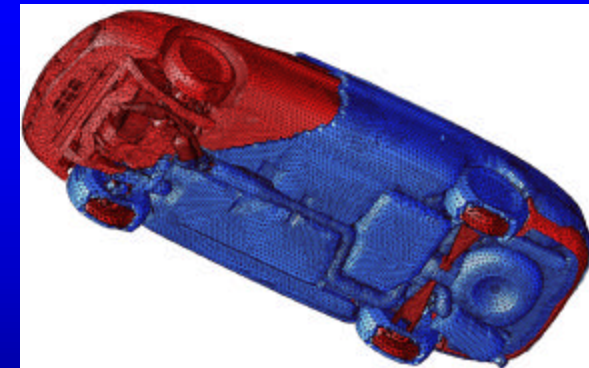
- **Overture** - high quality, predominantly structured meshes on complex CAD geometries (LLNL)
- Variational and Elliptic Grid Generators (ORNL, SNL)

- **Unstructured meshes**

- **AOMD** (RPI) - primarily tetrahedral meshes, boundary layer mesh generation, curved elements, AMR
- **CUBIT** (SNL) - primarily hexahedral meshes, automatic decomposition tools, common geometry module
- **NWGrid** (PNNL) - hybrid meshes using combined Delaunay, AMR and block structured algorithms
- **Frontier** (BNL) – interface front tracking



*Overture Mesh (LLNL)*



*MEGA  
Boundary  
Layer  
Mesh (RPI)*

# The Challenge

- These tools all meet particular needs, but
  - They do not interoperate to form hybrid, composite meshes
  - They cannot be interchanged easily in an application
- In general the technology requires too much software expertise from application scientists
  - Difficult to improve existing codes
  - Difficult to design and implement new codes

# Near and long term approach

Near term collaborations helps us understand application requirements ...

- *Near term*: deployment of current TSTT mesh and discretization capabilities by partnering with SciDAC applications
- *Long term*: development of interoperable software tools enabling
  - Rapid prototyping of new applications
  - Plug-and-play insertion of mesh and discretization technology through uniform software interfaces

... feeding into interface design of future software components

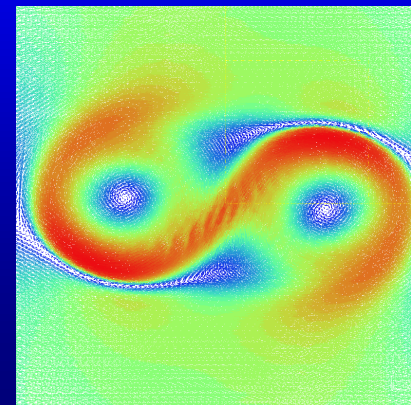
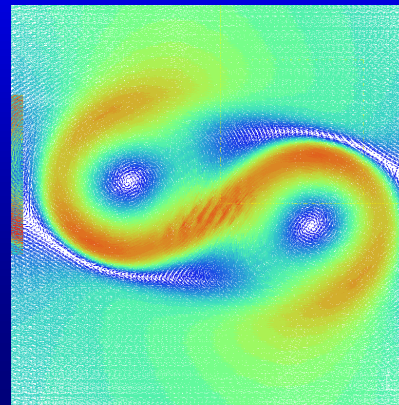
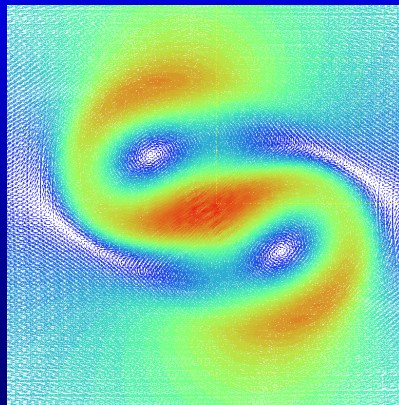
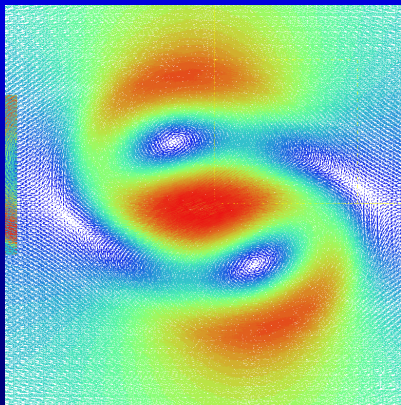


# Near Term Strategy

- Interact with SciDAC Applications. Develop working relationships in each application area by
  - Analyzing the needs of application scientists
  - Inserting existing TSTT technology
    - Provides a short-term impact for application scientists
    - Builds trust relationship
  - Developing new technologies for later insertion and new application development
- Key application areas: Fusion, Astrophysics, Accelerator Design, Climate

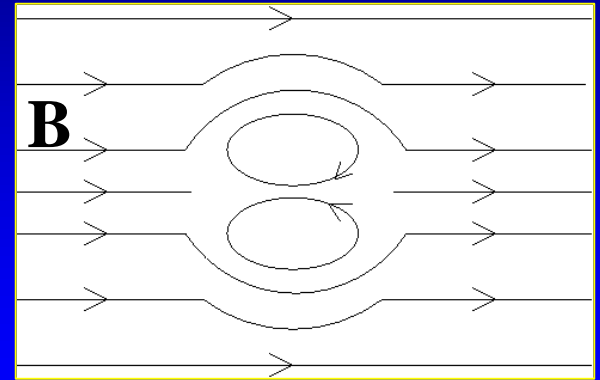
# High-Order FEM for Fusion

- High-order, adaptive finite element techniques for magneto-hydrodynamics
  - Fusion PI: Jardin/Strauss (PPPL)
  - TSTT PI: Shephard/Flaherty (RPI)
  - *Goal:* To test high-order and adaptive techniques; compare to existing linear FEM
  - *Progress:*
    - Initial results obtained for both potential and primitive variable mixed formulations for the 2D adipole vortex flow pattern
      - Two oppositely directed currents embedded in a constant magnetic field which holds them in an unstable equilibrium
      - They compress and rotate to align with magnetic field to reduce energy (see below)
    - Test of high-order and h-adaptive techniques available in Trellis to determine applicability to this problem
    - Quadratic and cubic results



# Example : Tilt Instability

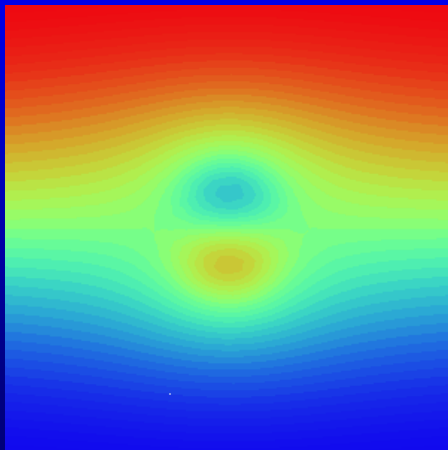
- Initial equilibrium consists of two oppositely directed currents embedded in a constant magnetic field
- Initial magnetic field ( $B$ ) is a dipole vortex
- Vortices are unstable to perturbations
- Kinetic energy grows like  $\exp(\gamma t)$
- Stream function formulation of MHD solved using stabilized finite element method



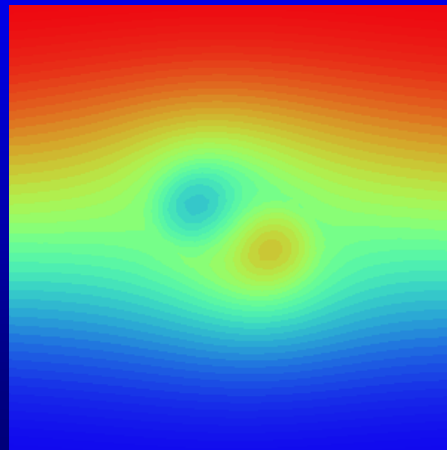
## Magnetic Flux ( $\psi$ )

$\mu = 0.005$ , order = 2 and mesh of 924 elements

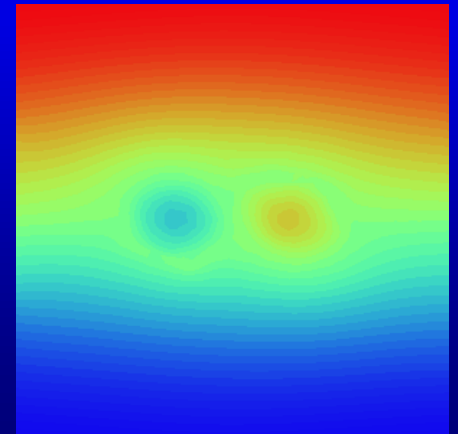
$t = 0$



$t = 5$

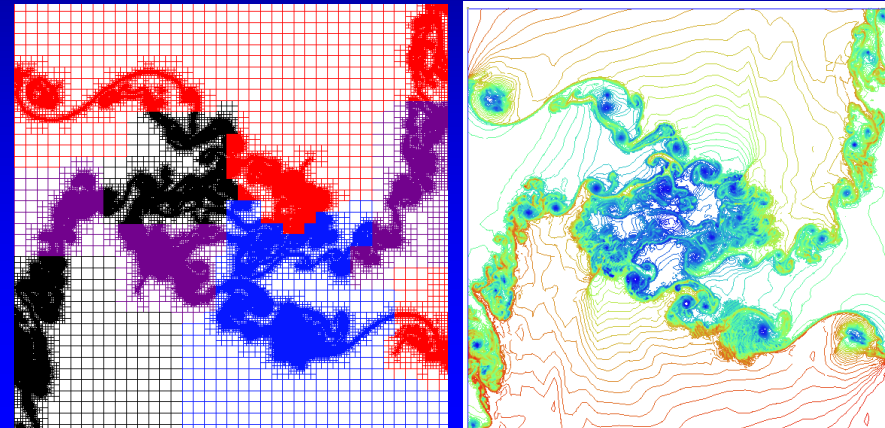


$t = 6$

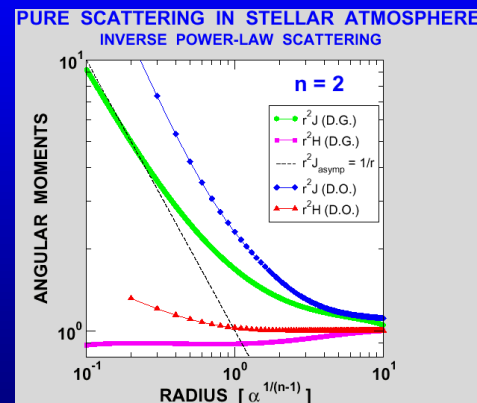


# Adaptive DG for Astrophysics

- Contact instabilities in hydrodynamics
  - Application PI: Bhattacharjee/Rosner (Iowa/UofC)
  - TSTT PI: Shephard (RPI)
  - *Goal*: to test h-p adaptive DG in hydrodynamics; compare to existing PPM
  - *Progress*: 3-D adaptive test to 256 processors have been done in Trellis for four contact Riemann problem
- Boltzman transport equations for neutrinos
  - Application PI: Mezzacappa (ORNL)
  - TSTT PI: de Almeida (ORNL)
  - *Goal*: to eliminate barriers imposed by discrete ordinates discretization (non-adaptive, computationally intensive) by developing a discontinuous Galerkin alternative
  - *Progress*: adaptive DG shows strong exponential decay, energy conservation, and outward peaking and gives better results than DOM



Adaptive mesh and density contours after structures have evolved. Colors on right mesh indicates processor assignment for this 4 processor case

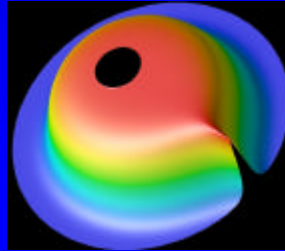
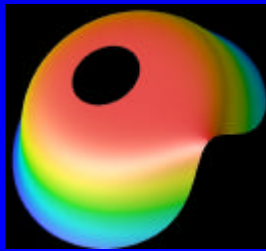
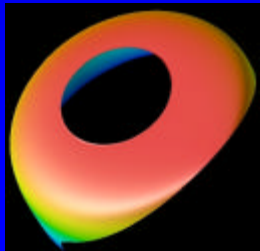
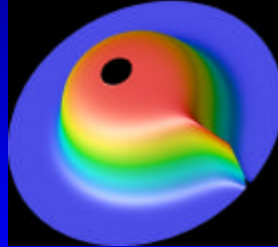
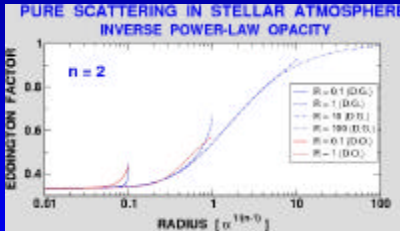
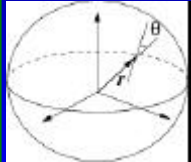


DOM does not reach asymptotic limit at large optical depth and does not conserve energy

Adaptivity in DGM provides more accuracy the slight loss of energy will be corrected

Mean Radiation Intensity (J); Net Energy Flux (H)

# SUPERNOVA RAD TRANSFER



## GOALS

Novel solution methods for neutrino Boltzmann transport as part of supernova simulation models

Faster, less memory consuming, and more accurate than current methods

## APPROACH

Discontinuous Galerkin method for hyperbolic Operator

Adaptive finite element of phase space

Splitting of hyperbolic and integral operators

Moment iteration

## ACCOMPLISHMENTS

Solution of the spherical Milne's problem and comparison against the Discrete Ordinate Method

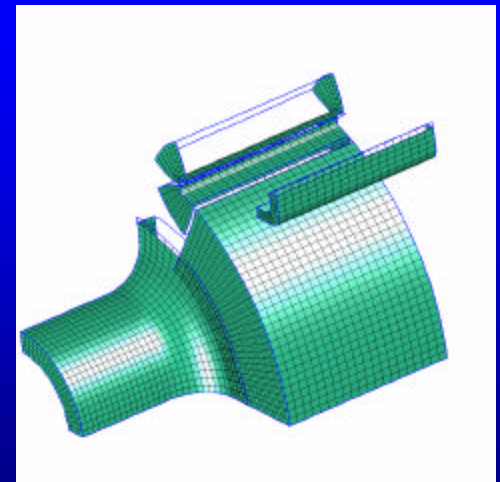
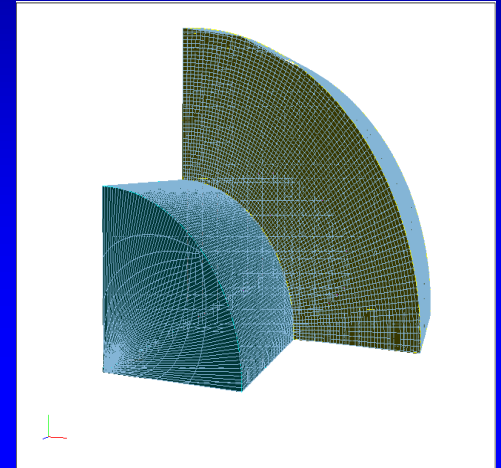
Proposed method captures all singularities

Faster and less memory consuming by one order of magnitude

Significantly more accurate

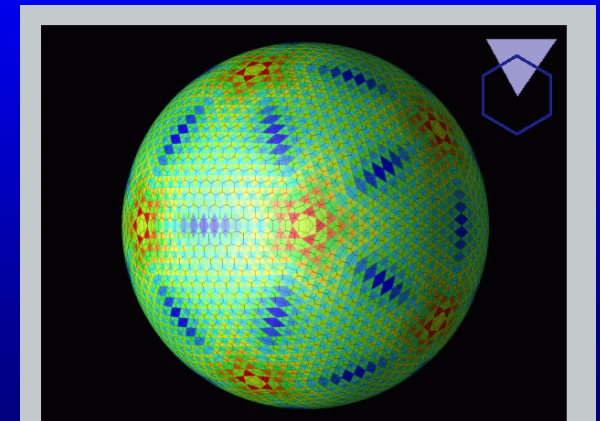
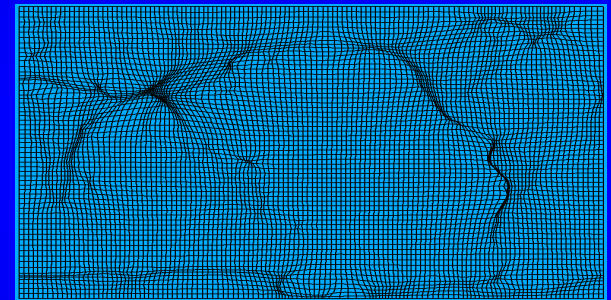
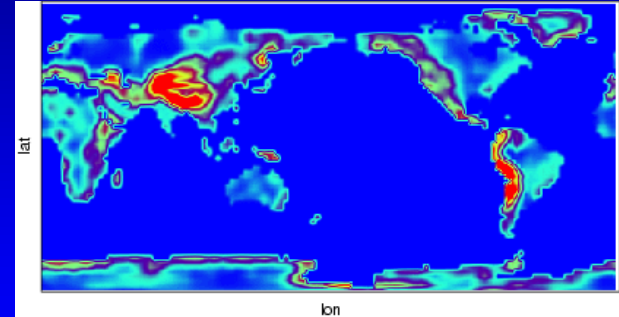
# Mesh Quality in Accelerator Design

- Understanding the effect of mesh quality on Tau3P
  - Application PI: Ko/Folwell (SLAC)
  - TSTT PI: Knupp (SNL), Henshaw (LLNL)
  - *Goal:* Determine the mesh quality factors that most affect stability of Tau3P and to devise discretization schemes to improve the stability of Tau3P without affecting long-time accuracy
  - *Progress:*
    - Systematic mesh quality analysis using CUBIT meshes revealed that run time varies by a factor of 3 from “best” to “worst” mesh and that smoothness and orthogonality are the most important factors
    - Analytically derived sufficient conditions on mesh quality for stability of discretization in Tau3P
    - Implemented basic Tau3P discretization strategy in Overture and analyzing feasibility of schemes for increasing the artificial diffusion



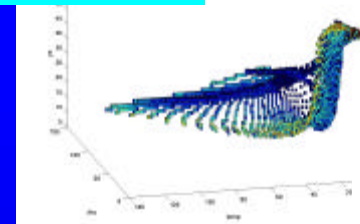
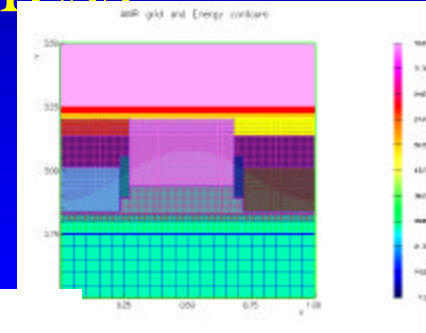
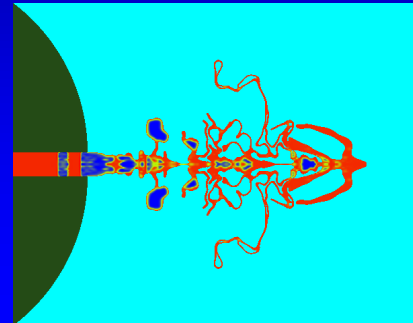
# Climate

- Adaptive gridding to minimize solution error
  - Application PI: Drake (ORNL)
  - TSTT PI: Khamayseh (ORNL)
  - *Goal:* Given an initial isotropic or anisotropic planar or surface mesh and a solution field with large gradient mountain heights, use solution based r-adaptation to minimize solution error
  - *Progress:* Proof of principle of meshing technologies demonstrated
- Geodesic mesh quality improvement
  - Application PI: Randall/Ringler (Colorado)
  - TSTT PI: Knupp (SNL)
  - *Goal:* Create smoothed geodesic grids to improve calculation accuracy
    - Plan to use early version of Mesquite to create smoothed grids with respect to element area and perform calculations with smoothed grids to determine effect in Fall '02

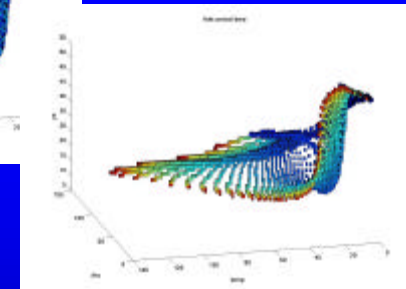


# Other examples where TSTT technology is helping near-term application progress

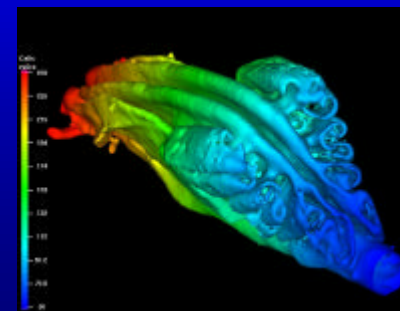
- Front tracking and adaptive techniques in Frontier and Overture for modeling of the breakup of a diesel fuel jet into spray (Argonne/BNL)
- 3D caching schemes to avoid redundant, costly evaluations of scattering kernels in phase space in astrophysics calculations (ORNL/ORNL)
- Mesh-based schemes for computational biology applications such as rat olfactory systems and human lungs (PNNL/PNNL)
- Low-order discretization schemes used as effective preconditioners in Climate applications (Colorado/ANL)



Access pattern :red is more frequent



Access sequence: red is accessed late in simulation



# Long Term Strategy

- Create interoperable meshing and discretization components
  - Common interfaces for mesh query and modification
  - Initial design will account for interoperability at all levels
  - Encapsulate existing TSTT software tools into CCA-compliant components for plug and play
- Develop new technologies as needed to enable interoperability
  - High-level discretization library
  - Mesh quality improvement for hybrid meshes
  - Terascale algorithms for adaptivity, load balancing, interpolation

# Low Level Access

- Access the mesh through the individual components
- For example
  - element-by-element access to mesh components
  - fortran-callable routines that return interpolation coefficients at a single point (or array of points)
- Facilitates incorporation into existing applications

# High Level Access

- Operate on the mesh components as though they were a single mesh object
  - Discretization operators
  - Mesh modifications
    - Mesh quality improvement
    - Refinement/coarsening
  - Error estimation
  - Multilevel data transfer
- Prototypes provided by Overture and Trellis frameworks
- Enables rapid development of new mesh-based applications

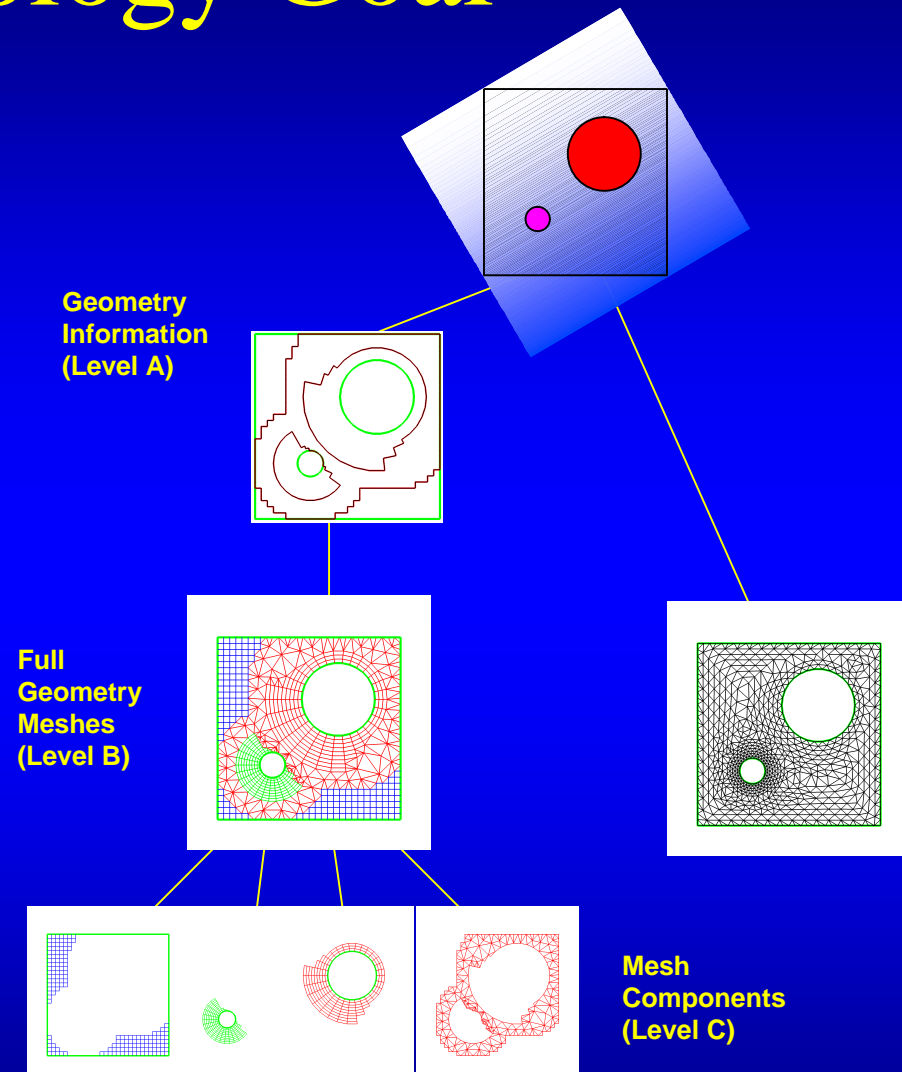
# TSTT Technology Goal

**To provide *interchangeable and interoperable* access to different mesh management and discretization strategies**

- Ease experimentation with different technologies
- Combine technologies together for hybrid solution techniques

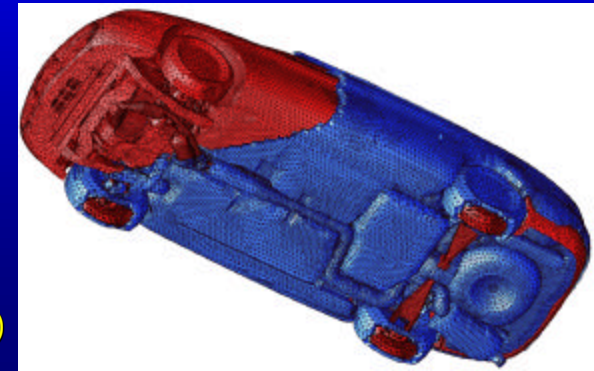
## The Data Hierarchy

- **Level A: Geometric description of the domain**
  - provides a common frame of reference for all tools
  - facilitates multilevel solvers
  - facilitates transfer of information in discretizations
- **Level B: Full geometry hybrid meshes**
  - mesh components
  - communication mechanisms that link them (key new research area)
  - allows structured and unstructured meshes to be combined in a single computation
- **Level C: Mesh Components**



# The Challenge

- TSTT brings together many meshing and discretization tools
  - Structured Grids: Overture, ORNL variational techniques
  - Unstructured Meshes: AOMD, CUBIT, NWGrid, Frontier
- These tools all meet particular needs, but
  - They do not interoperate to form hybrid, composite meshes
  - They cannot be easily interchanged in an application
- In general the technology requires too much software expertise from application scientists
  - Difficult to improve existing codes
  - Difficult to design and implement new codes



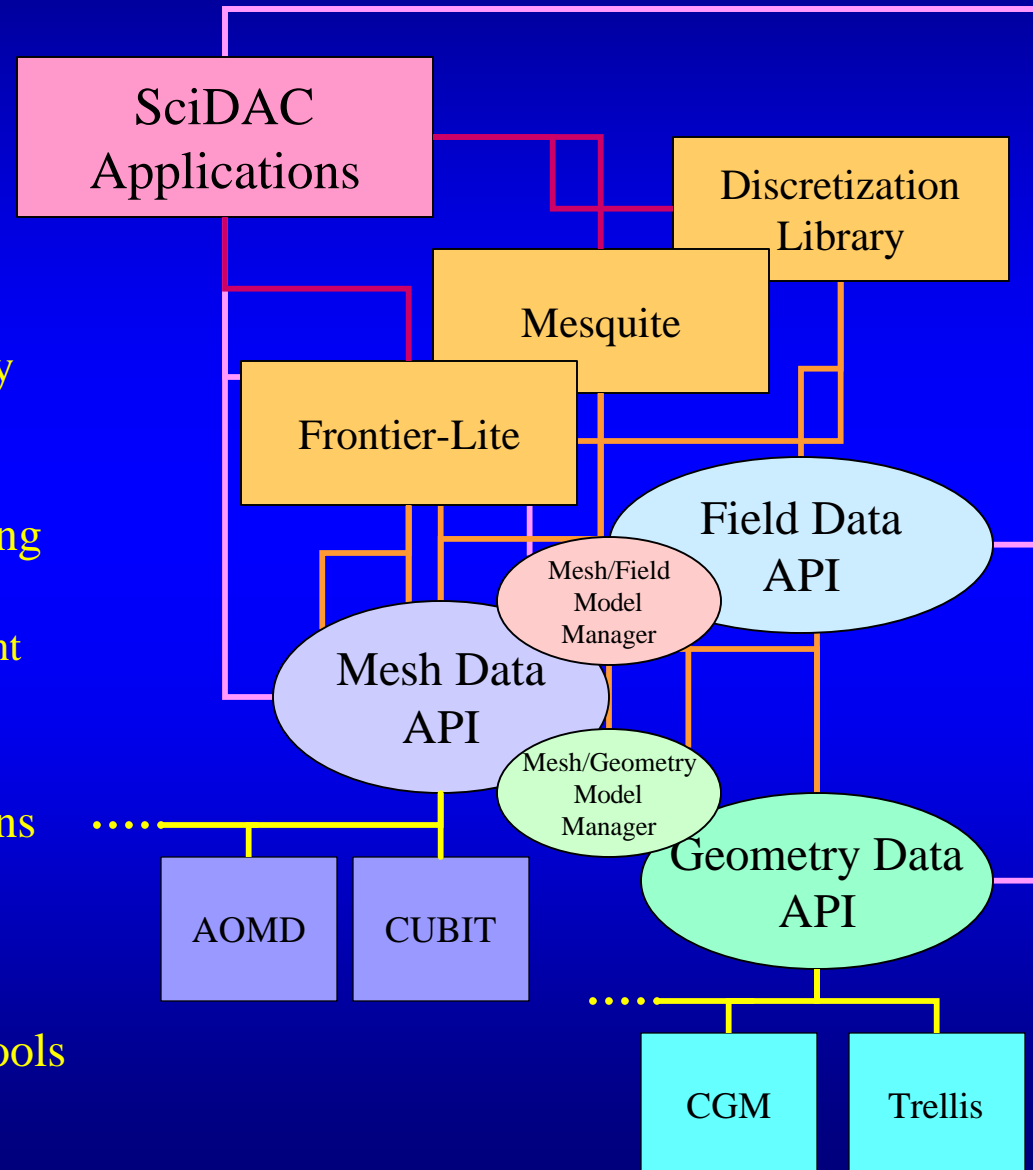
MEGA Boundary Layer Mesh (RPI)

# Technology Development Strategy

- Create plug-and-play meshing and discretization components from existing technologies
  - Define common interfaces for mesh query and modification
  - Showcase interoperability goal through one-to-one demonstrations
  - Encapsulate existing TSTT software tools into CCA-compliant components for plug and play
- Develop new technologies as needed to enable interoperability
  - Mesh quality improvement for hybrid meshes
  - High-level discretization library
  - Terascale algorithms for adaptivity, load balancing, interpolation

# Interoperability Development Plan

- Define interfaces for
  - Mesh Data
  - Geometry Data
  - Field Data
  - Data Model Managers
- Wrap existing TSTT tools to comply with these interfaces
- Create new tools that use these interfaces to work with the underlying infrastructures interchangeably
  - Mesquite mesh quality improvement
  - Discretization Library
  - Frontier-Lite
- Use these tools to impact applications
- Use TSTT interfaces directly in applications to allow plug-and-play experimentation
- Use TSTT interfaces to use TSTT tools interoperably



# Interoperability: TSTT Interface Specification

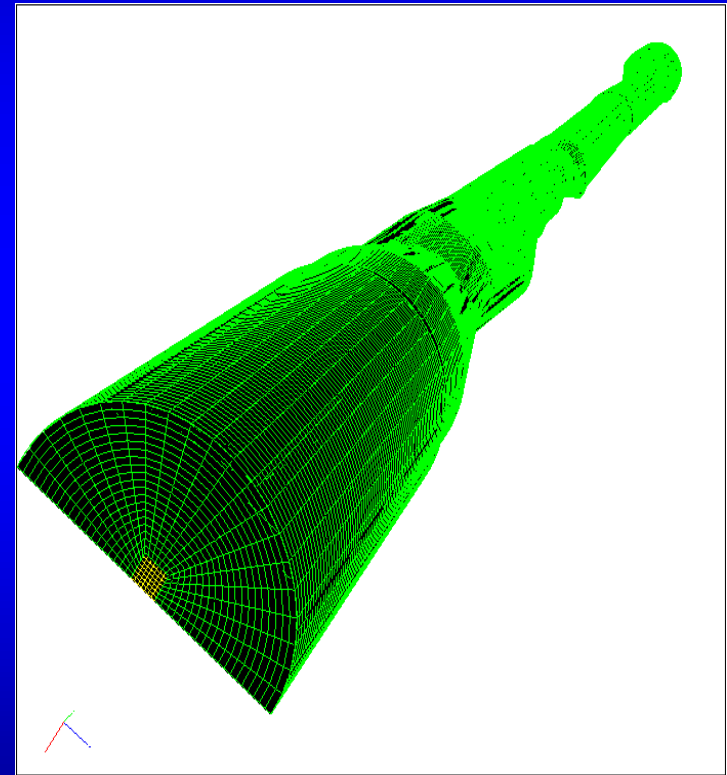
- **Philosophy**
  - Create a small sets of interfaces that existing packages can support
  - Be data structure neutral
  - Balance performance and flexibility
  - Work with a large tool provider and application community to ensure applicability
- **Status**
  - Interfaces mesh geometry and topology well underway
    - Mesh Query
    - Entity Sets (subsetting)
    - Modifiable Meshes (a basic form of adaptive meshing)
  - Prototype interfaces for geometry and field data
  - Prototype interface for the mesh/geometry data model manager
    - Classification
  - Prototype implementations
    - AOMD, Overture, NWGrid, MDB/CUBIT
    - C, C++, and Fortran language interoperability through SIDL/Babel (CCA)
  - Used in Mesquite for interchangeability
  - Point of Contact: L. Freitag

# One-to-One Tool Interoperability

- Showcases impact of interoperable tools on applications
- Frontier (BNL/SUNY SB) - Overture (LLNL) Merge
  - Combines adaptive mesh technology with Front-tracking
  - Initial merge complete and used in simulations
  - Next step is to parallelize adaptive schemes for a scalable solution strategy
  - Will create a TSTT-compliant Frontier-Lite library for use with other TSTT mesh management tools (NWGrid, AOMD)
  - Point of Contact: X. Li
- NWGrid (PNNL) - Opt-MS (ANL)
  - Incorporates previously developed mesh quality improvement tools
  - Uses a CCA interfaces for dynamic plug and play
  - Migration to Mesquite via the TSTT interface planned for Fall 03
  - Point of Contact: H. Trease

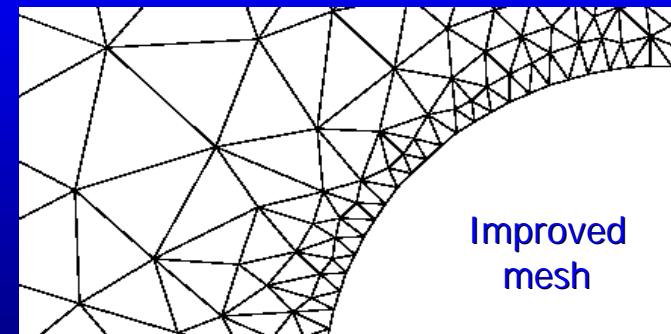
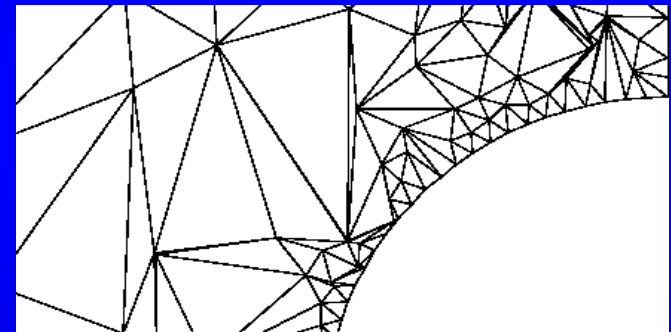
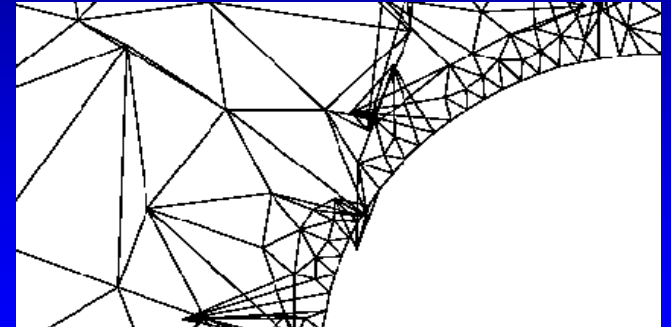
# New TSTT Tools: Mesh Quality Improvement

- Goal: To provide a stand-alone tool for mesh quality improvement
  - hybrid, component based meshes
  - development of quality metrics for high order methods
  - a posteriori quality control using error estimators
- Methods
  - optimization-based smoothing and untangling (based on Opt-MS and CUBIT algorithms)
  - reconnection schemes
- Status
  - Initial design complete and implemented
  - Tri, tet, quad, hex, and hybrid meshes
  - Several quality metrics and objective functions
  - Conjugate Gradient, Newton, Active Set solvers
- SciDAC Impact
  - SLAC mesh quality improvement
  - Geodesic grids in climate
  - Integrated with CUBIT, AOMD via TSTT interface
- Points of Contact: P. Knupp, L. Freitag



# Mesh Quality Improvement

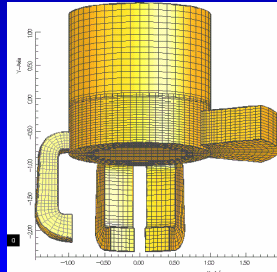
- *Goal:* To provide a stand-alone tool for mesh quality improvement
  - hybrid, component based meshes
  - development of quality metrics for high order methods
  - a posteriori quality control using error estimators
- *Methods*
  - optimization-based smoothing and untangling (based on Opt-MS and CUBIT algorithms)
  - reconnection schemes
- *Status*
  - Prototype designed and most classes implemented for a simple optimization algorithm
  - Opt-MS and CUBIT algorithms inserted this summer
  - Built on TSTT interface
- *SciDAC Application Impact*
  - SLAC mesh quality improvement
  - Geodesic grids in climate
  - Integrated with CUBIT, NWgrid, Overture, AOMD



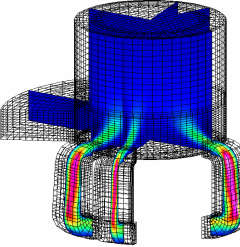
# New TSTT Tools: Discretization Library

- *Observation:* Complexities of using high-order methods on adaptively evolving grids has hampered their widespread use
  - Tedious low level dependence on grid infrastructure
  - A source of subtle bugs during development
  - Bottleneck to interoperability of applications with different discretization strategies
  - Difficult to implement in general way while maintaining optimal performance
- Result has been a use of sub-optimal strategies or lengthy implementation periods
- *TSTT Goal:* to eliminate these barriers by developing a *Discretization Library*

# Example: Overture prototype



Incompressible Navier-Stokes v  
t = 0.90 dt = 0.36E-02 nu = 0.1000



Min = -0.18E+00 Max = 0.20E+01

```
CompositeGrid cg;  
floatCompositeGridFunction u, v, w;
```

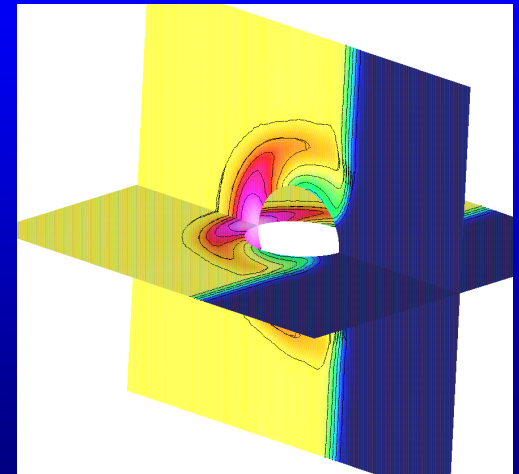
*Differentiation Operators*

```
v = u.y();  
w = u.laplacian();
```

*Visualize grid  
and data*

```
Plotstuff ps;  
ps.plot (cg);  
ps.contour (w);
```

Trellis (RPI) provides similar capability for  
finite-element method



# Discretization Library Functionality and Status

- Planned functionality
  - Mathematical operators will be implemented
    - $+$ ,  $-$ ,  $*$ ,  $/$ , interpolation, prolongation, div, grad, curl, etc
    - Both strong and weak (variational) forms of operators when applicable
  - Many discretization strategies will be available
    - Emphasize high-order and variable-order methods
    - Extensive library of boundary condition operators
  - The interface will be independent of the underlying mesh by using the TSTT interface
- Status:
  - Existing schemes decoupled from their frameworks
    - Finite Element, Discontinuous Galerkin from Trellis; Finite Volume from Overture; Spectral Elements from Nek5000
  - Working to create a set of common interfaces for application use
  - Exploring the issues associated with hybrid solution strategies (mixed element meshes, mixed discretization solution techniques)
  - Point of Contact: D. Brown

# TSTT ISIC Collaborations

- TOPS: (PI: Keyes)
  - provide mesh representations for multilevel techniques
  - co-develop well-defined interfaces to ensure that the meshes and discretization strategies will be interoperable with solution software
- APDEC: (PI: Colella)
  - provide mesh generation technologies via Overture
  - co-develop common interfaces for block structured AMR strategies
- CCA: (PI: Armstrong)
  - co-develop common interfaces for mesh and field data
  - create CCA-compliant mesh components and provide them in the CCA component repository
  - explore the role of the component model in the composition of numerous discrete operators
- Performance: (PI: Bailey)
  - we will use *ROSE* preprocessor to develop highly-tuned discretization libraries
  - TSTT will provide benchmarks and a testing environment for developments in the performance ISIC

# Summary

The TSTT Center focuses on interoperable meshing and discretization strategies on complex geometries

- Short term impact through technology insertion into existing SciDAC applications
- Long term impact through the development of
  - a common mesh interface and interoperable and interchangeable mesh components
  - new technologies that facilitate the use of hybrid meshes
- Working with SciDAC ISICs to ensure applicability of tools and interfaces

# Contact Information

- TSTT Web Site: [www.tstt-scidac.org](http://www.tstt-scidac.org)
- David Brown: [dlb@llnl.gov](mailto:dlb@llnl.gov)
- Lori Freitag: [ladiach@sandia.gov](mailto:ladiach@sandia.gov)
- Jim Glimm: [glimm@ams.sunysb.edu](mailto:glimm@ams.sunysb.edu)